



Atomic and Molecular Design of Materials for Sustainable Energy Storage Solutions

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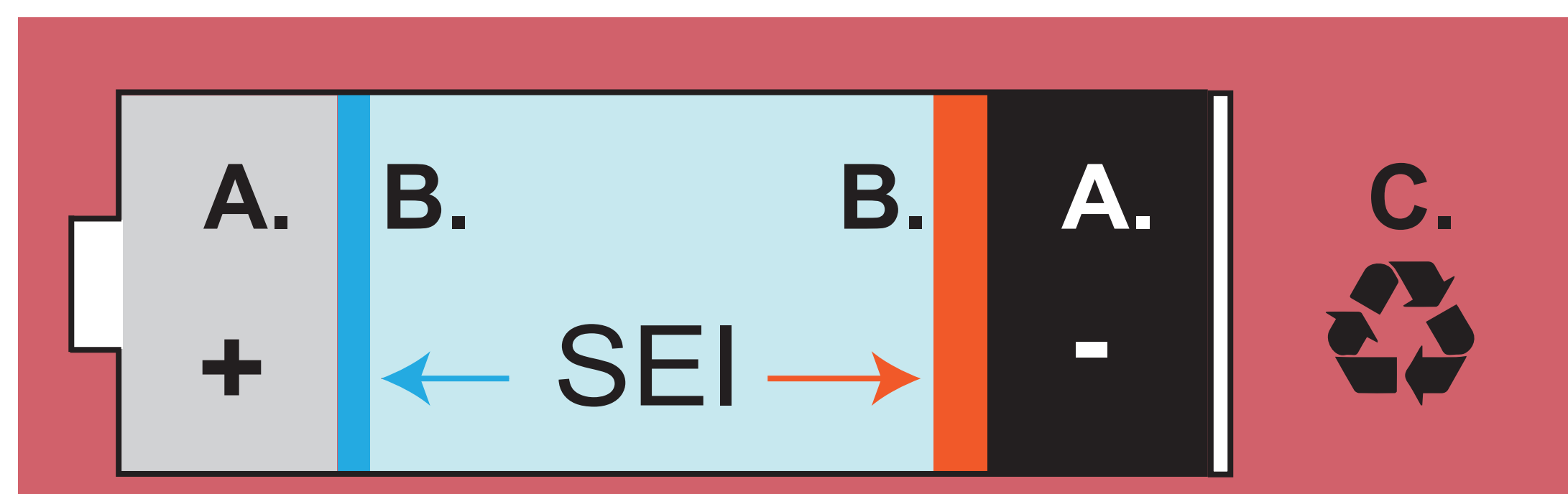
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Summary of Group

Computational scientists working closely with **experiments** to address **sustainability** challenges in **energy storage** and the **environment**.

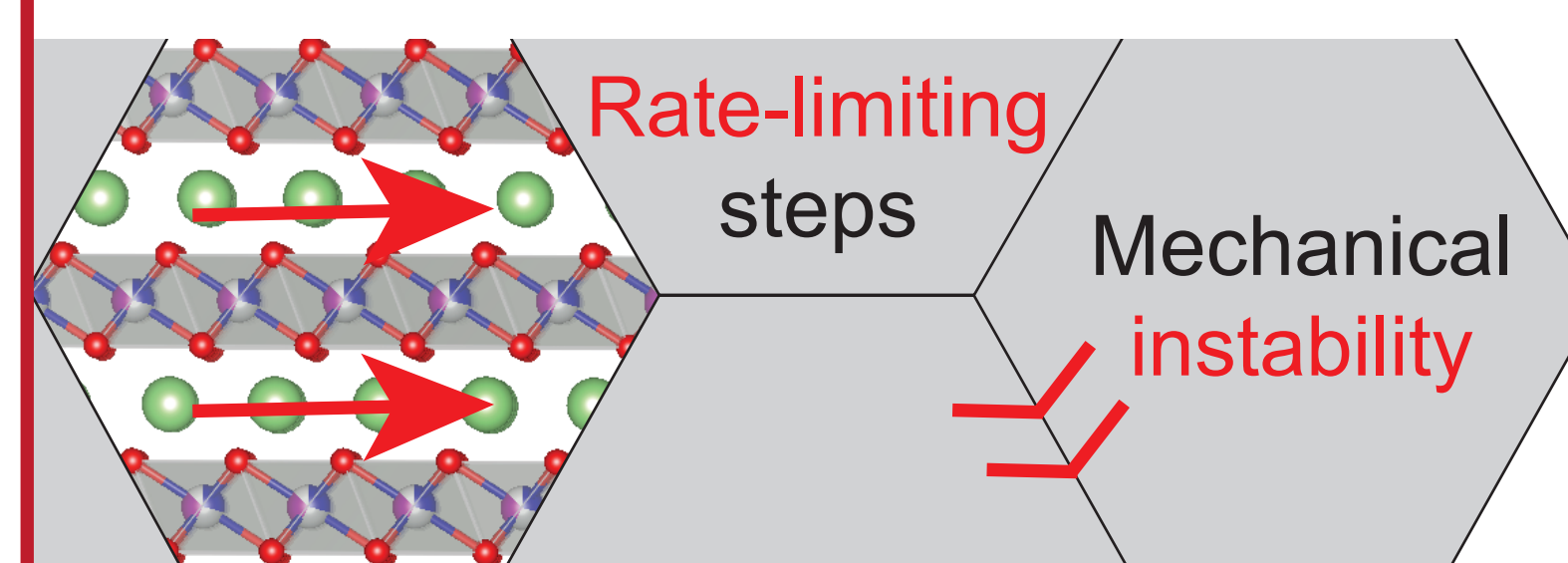
Electrochemistry | First-principles | Machine Learning



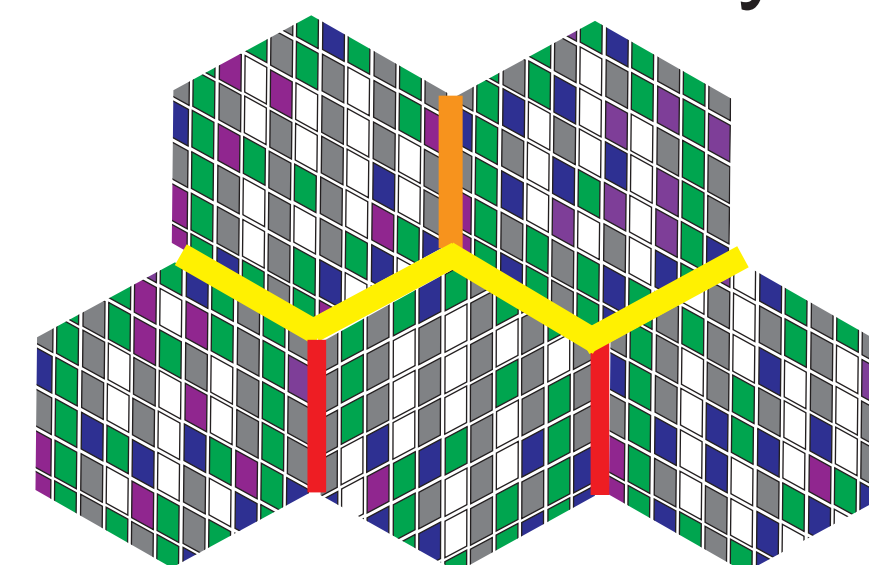
Research Plan & Potential Funding



A. How does polycrystal structure control battery performance?



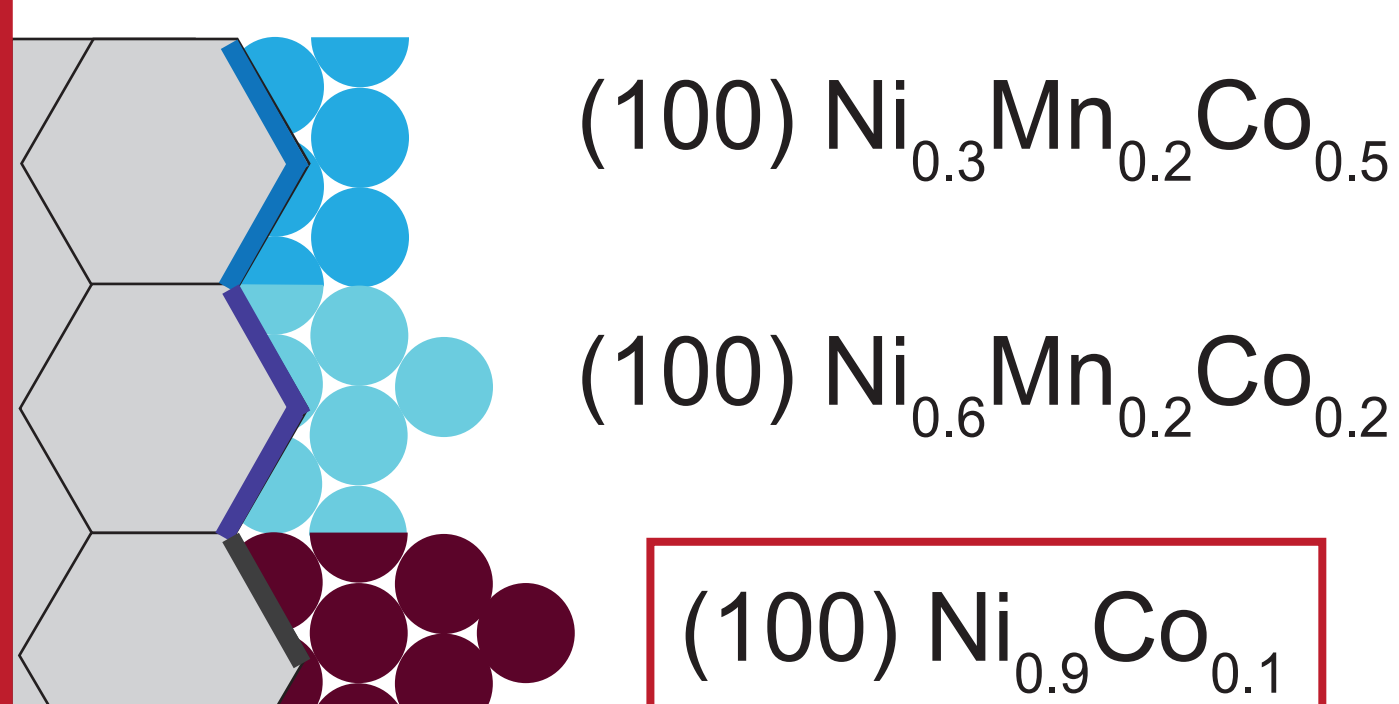
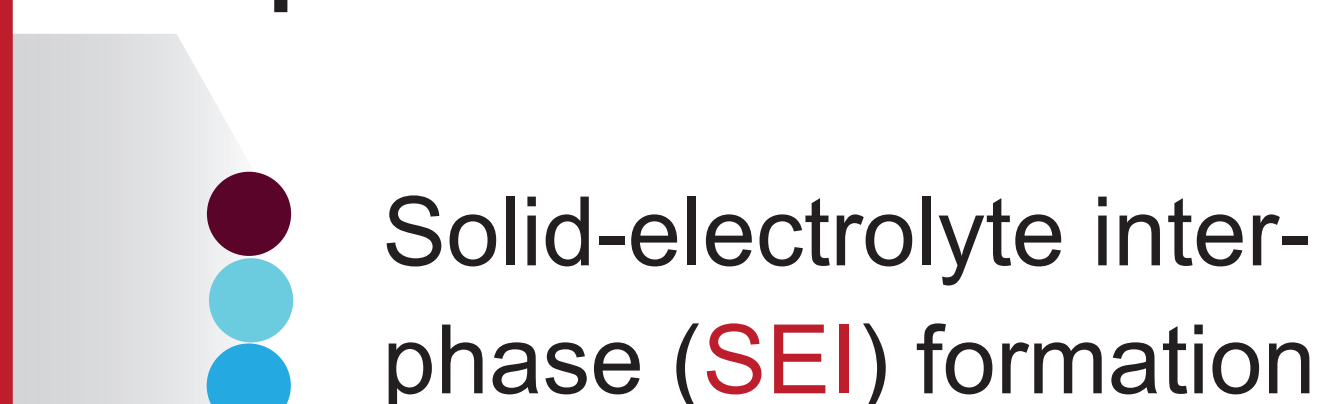
Design principles for ion transport and mechanical stability



All-atom electrochemical models

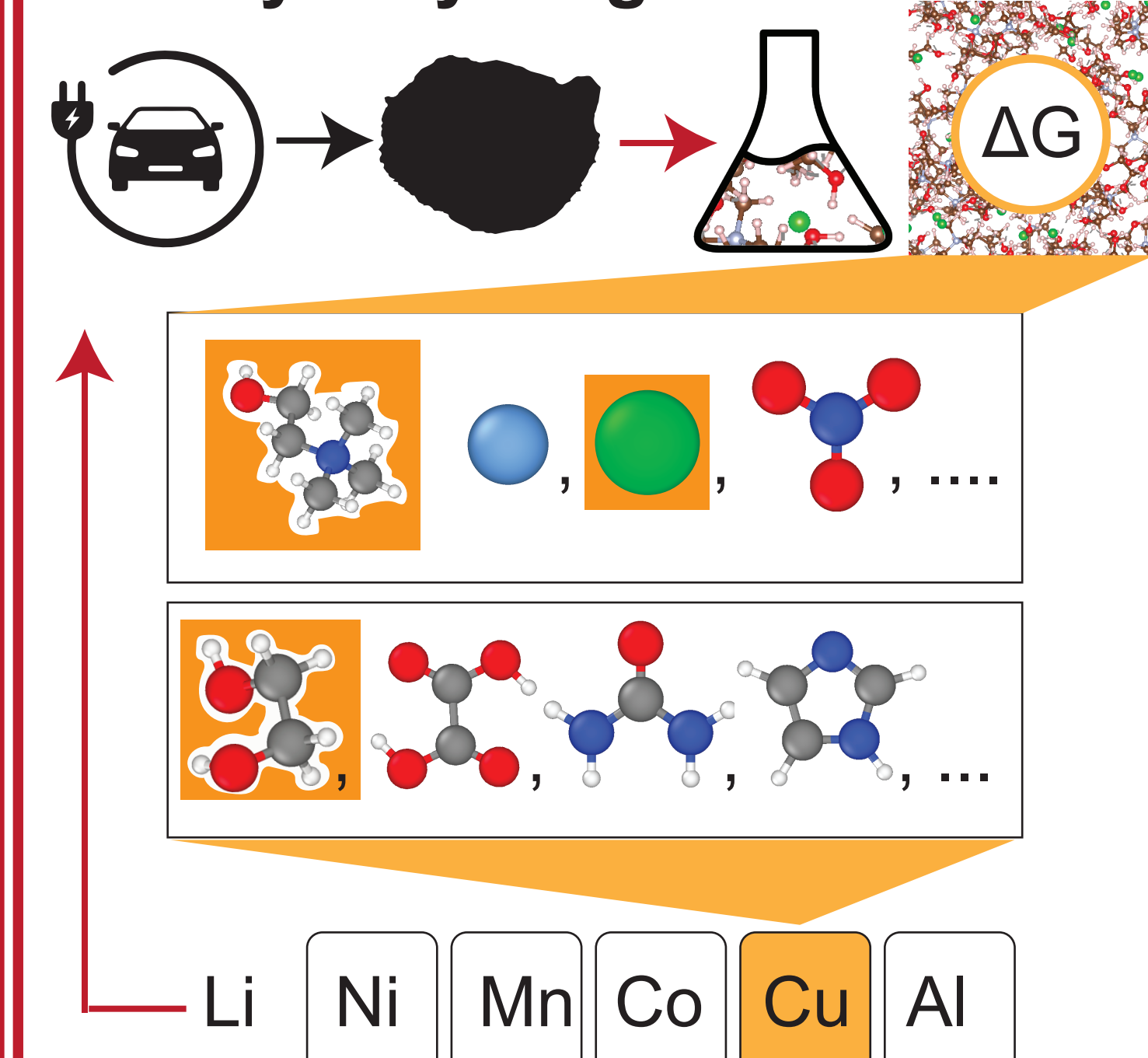
1. **J.H. Yang** & G. Ceder, Adv. Energy Mater. 13(4), (2023).
2. **J.H. Yang**, T. Chen, L. Barroso-Luque, Z. Jadidi, G. Ceder, npj Comput. Mater. 8(1), (2022).
3. **J.H. Yang***, J.C. Kim*, D.-H. Kwon*, ..., G. Ceder, Adv. Energy Mater. 10(31), (2020).

B. How do critical surfaces dictate reactivity and interphase formation?



1. **J.H. Yang**, D. A. Kitchaev, G. Ceder, Phys. Rev. B 100(3), (2019).
2. L. Barroso-Luque, **J.H. Yang**, F. Xie, T. Chen, R. L. Kam, ..., G. Ceder, JOSS 7(77), (2022).
3. **J.H. Yang**, A. W-S. Ooi, Z. A. Goodwin, ..., A.-H.A. Park, B.Kozinsky, *in preparation*.

C. How should we design solvents for tunable battery recycling?



1. **J.H. Yang**, V. Gharakhanyan, T. Gadhiya, A.Holiday, U.S. Patent App (filed Oct. 17, 2022).
2. **J.H. Yang**, H. Kim, G. Ceder, Molecules 26(11), (2020).
3. D. Morgan, B. Kozinsky, V. Honavar, **J.H. Yang**, ..., *in preparation*.

Education, Awards, and Proposals

Environmental Fellow, Harvard University
Environmental Fellowship (2022-2024),
 NextProf Nexus (2023)

Ph.D. (2022), Materials Science & Eng., UC Berkeley
NDSEG Fellowship (2016-2019),
 UC Berkeley MSE Rising Star Scholarship (2016)

B.S., (2016), Materials Science & Eng., CMU
 Tau Beta Pi, College Honors, University Honors,
 Senior Leadership Award (2016),
SRC Undergraduate Fellowship (2014-2016)

Teaching Experience

Thermodynamics | Graduate Student Instructor, UC Berkeley MSE, Fall 2019
 Peer Tutor, CMU MSE, Jan. 2013-May 2016

Programming & Computing | Invited Lecturer on DFT, CMU Elect. & Comput. Eng, Spring 2020
 Intro. to Python Course Assistant, CMU SCS, Fall 2015

Energy Storage | Invited Lecturer on Batteries, Harvard Env. Sci. & Public Policy, Spring 2024

References & Contact Information

Prof. Gerbrand Ceder, UC Berkeley MSE
 Prof. Boris Kozinsky, Harvard SEAS
 Dean Ah-Hyung Alissa Park, UCLA CBE
 Dr. Alexander Holiday, X (formerly Google X)
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Planned Outreach and Examples of Service

Engage with local middle and high schools
 (A. Berkeley High School SEED program)
Initiate and orchestrate DEIB opportunities
 (B. NextProf Nexus 2023)
Lead national conversations
 (C. ACS 2023 "What to Expect in Grad. School")

